

Author index

Abad-Zapatero,C. 865
Abagyan,R. 249
Adams,G.P. 301
Adams,J.A. 609
Adib-Conquy,M. 859
Adman,E.T. 153
Adzhubei,A.A. 615
Aert,R. 159
Akutsu,N. 39
Albrechtsen,B. 1063
Alexander,R.S. 975
Alftman,K. 725
Amadei,A. 1129
Amati,V. 403
Ammendola,S. 31
Anderson,F. 1189
Anderson,H.W. 1063
Appelt,K. 677
Åqvist,J. 1137
Aramaki,H. 1259
Argos,P. 21,1011
Atkinson,H.J. 1303
Avrameas,S. 859

Baase,W.A. 1017
Baker,K.C. 59
Baker,P.J. 147
Bakker,A.H.F. 293, 1295
Baláz,S. 809
Banerjee, S. 1189
Barnett,J. 275
Bayley,H. 491
Beato,M. 71
Benhabiles,N. 829
Benner,S.A. 457
Bennett,G.L. 1057
Bennett,S. 91
Beppu,T. 153
Berendsen,H.J.C. 1129
Betts,A.H. 593
Beveridge,A.J. 135
Bi,R.-C. 211
Björkstén,J. 5
Blättler,W.A. 481
Boberg,J. 501, 505
Bohr,H. 389
Bookman,M.A. 301
Boutonnet,N.S. 647
Brady,J.W. 1145
Brasseur,R. 829
Brem,R. 1205
Brennan,C. 865
Brenner,S.E. 319
Briggs,G.S. 59
Brinkmann,U. 1323
Britton,K.L. 147
Brown,A.M. 397
Brukner,I. 283

Cambria,A. 551
Carter,D.C. 471
Carter,P. 1057
Cattaneo,A. 403
Chan,C.M.W. 193
Chan,H.S. 1205
Chao,Y. 211
Chen,H.-m. 575
Chen,L. 865, 1049
Chen,M.-J. 1233
Chiaraluce,R. 1287
Chiu,C.Y. 463
Chou,K.-C. 425

Christianson,D.W. 975
Christodoulou,C. 859
Chu,N.-M. 211
Clark,B.F.C. 1267
Collins,J. 45
Collura,V.P. 1197
Colotti,G. 593
Connerton,I.F. 59
Consalvi,V. 1287
Coutinho,P. 1049
Craik,C.S. 275
Cummings,N.J. 59
Cygler,M. 835

Daggett,V. 1117
Danson,M.J. 583
Davies,P.L. 843
De Benedetti,P.G. 557
De Maeyer,M. 815
de Vlieg,J. 21
de Vos,W.M. 117, 1287
Dealwis,C.G. 865
Declerck,N. 1029
Degtyarenko,K.N. 737
Delagrange,S. 237
delCardayré,S.B. 261
DeLisi,C. 1081
Demetrius,L. 791
Desideri,A. 551
Desmet,J. 815
Dhopke,V.M. 315
Dill,K.A. 769, 1205
Doi,H. 1171
Dunkel,R. 71

Eggen,R.I.L. 1287
Egmond,M.R. 21
Eisenberg,D. 627
Elce,J.S. 843
Eldridge,M.D. 1197
Elliott,G. 471
Ely,K.R. 823
Emahazion,T. 1163
Engberg,J. 1063
Engel,P.C. 147
Eroshkin,A.M. 167

Fand,I. 301
Fanelli,F. 557
Farber,G.K. 1189
Farkas,Ö. 925
Fastrez,J. 451
Fernández,J.A. 1253
Fierke,C.A. 975
Findlay,J.B.C. 1129
Finkelstein,A.V. 207, 883
Firth,M.A. 1197
Fischer,D. 981
Flanagan,K. 109
Ford,C. 575, 1049
Fox,T. 53
Francis,D.M. 193
Freedman,R.B. 59
Freer,S.T. 677
Fu,Z.-Q. 1233
Fujita,I. 935
Fuxreiter,M. 925

Gaillardin,C. 1029
Gallet,X. 829
Galvano,M. 551
Galzitskaya,O.V. 883

Garnier,J. 1029
Gauthier,S. 843
Geerling,A.C.M. 1287
Gershoni,J.M. 143, 717
Gerstein,M. 319, 329
Gilbert,M. 859
Gileva,I.P. 167
Gish,G. 609
Gö,N. 353
Godzik,A. 409
Goffin,V. 1215
Goldmacher,V.S. 481
Goldman,E.R. 237
Goldstein,R.A. 641
Goodenough,P.W. 59
Goodenow,J.M. 109
Goormaghtigh,E. 249
Goraj,K. 249
Gould,H.J. 193
Griffin,J.H. 1253
Guild,B.C. 481

Hansen,L.K. 379
Hansson,T. 1137
Hara,T. 711
Hardman,K.D. 749
Harrison,R.W. 1233
Hartley,R.W. 497
Hashimoto,Y. 1023
Hayashi,Y. 763
Hecht,H.-J. 45
Hegadorn,C. 843
Heimstad,E.S. 379
Hemminki,A. 185
Henklein,P. 471
Henneke,C.M. 13
Henry,A.J. 193
Heringa,J. 21
Herzberg,O. 1275
Hide,M. 193
Ho,J.X. 471
Hoffrén,A.-M. 185, 443
Höhne,W. 471
Holewa,B. 733
Horinouchi,S. 153
Houbrechts,A. 249
Hough,D.W. 583
Houston,L.L. 301
Howard,A.J. 749
Hubbard,S.J. 1011
Hudziak,R.M. 301
Hunter,M.J. 1177
Huston,J.S. 301
Hwang,J.-K. 363

Imamura,M. 1171
Imberty,A. 699
Imoto,T. 201, 1023
Incani,O. 31
Ippolito,J.A. 975
Ishino,Y. 1171
Islam,S.A. 513

Janacek,S. 809
Jespers,L. 451
Jin,D. 301
Johansen,L.K. 1063
Johnson,M.S. 873
Joseph-McCarthy,D. 1103
Joyet,P. 1029
Jung,S.-H. 1323

Kadono,S. 763
Kamynina, T.P. 167
Kanppik,A. 81
Karginova,E.A. 167
Karplus,M. 1103
Karshikoff,A. 243
Katinger,D. 471
Kato,H. 711
Kato,I. 1171
Kaufman,S.E. 463
Kawaguchi,J. 763
Keeling,K. 471
Keller,D.A. 893
Kiefer,L.L. 975
Kirschner,K. 535
Klein-Hitpaß,L. 733
Klimenko,L.V. 63
Knudsen,C.R. 1267
Kodandapani,R. 823
Koga,H. 201
Kolinski,A. 225
Komeiji,Y. 935
Komives,E.A. 1177
Koshi,J.M. 641
Kramer,A. 471
Krek,C.E. 481
Kretsinger,R.H. 63
Kuijpers,O.P. 117
Kukimoto,M. 153
Kumugai,I. 1153
Kunicki,T.J. 823
Kurochkina,N. 437
Kuroda,Y. 97
Kuwajima,K. 1153

Ladino,C.A. 481
Laminet,A.A. 301
Lamproye,A. 249
Laramée,L. 835
Laskowski,R.A. 127
Lasters,I. 815
Laughton,C.A. 615
Lebbink,J.H.G. 1287
Lebedev,L.R. 167
Lee,B. 437, 1323
Lee,D.-H. 91
Leung,R. 275
Lewin,M. 829
Li,A. 1117
Li,J. 1197
Liao,W.-F. 363
Lim,C. 565
Linacre,J. 527
Liu,S. 301
Lomakin,A.S. 167
Lorenz,P. 733
Luo,J. 513

Mackay,G.A. 193
Maeda,Y. 201
Maggiore,G.M. 425
Mainfroid,V. 249
Mäkinen,M.-L. 185
Manchester,J.I. 801
Mandecki,W. 865
Mannervik,B. 1163
Marcus,E. 893
Marino,M. 551
Marotti,K.R. 293
Martial,J.A. 249, 1215
Martin,A.C.R. 389, 1093
Martin,S. 147

Author index

Mason,P. 53
 Matsushima,N. 63
 Matthews,B.W. 1017
 May,A.C.W. 873
 McCommon,J.A. 397, 663, 915
 McCartney,J.E. 301
 McDonald,I.K. 217
 McDonald,S.M. 915
 McGlone,M.L. 609
 McPherson,M.J. 1303
 Medvedkin,V.N. 63
 Meininger,D.P. 1177
 Mele,A. 31
 Menziani,M.C. 557
 Milik,M. 225
 Min,H.Y. 463
 Mitin,Y.V. 63
 Miyazawa,S. 999
 Mizuguchi,K. 353
 Mordenti,J. 1057
 Moreau,B. 249
 Moriyama,H. 763
 Mort,J.S. 53
 Mucovic,M. 497
 Muir,J.M. 583
 Mullenbach,G.T. 463
 Muro,M. 39
 Murphy,J.R. 1317
 Murray,C.W. 1197

Nagaraj,R. 315
 Nair,S.K. 975
 Nakayama,S. 63
 Nakhei,H. 733
 Náray-Szabó,G. 925
 Negro,A. 175
 Neidle,S. 615
 Niermann,T. 535
 Nieuwenbroek,N.M.E. 1295
 Nikolov,Z. 1049
 Nilsson,B. 601
 Nilsson,J. 601
 Nishioka,T. 711, 1075
 Nishiyama,M. 153
 Nord,K. 601
 Nosoh,Y. 39
 Nugel,E. 471
 Numata,K. 39, 763
 Nussinov,R. 981
 Nygren,P.-Å. 601

O'Connor,J. 1243
 Ochagavia,M.-E. 647
 Oda,J. 711, 1075
 Ohnuki,T. 153
 Okoniewska,M. 835
 Ollis,D.L. 135
 Onodera,K. 763
 Ophir,R. 143
 Oppermann,H. 301
 Ornstein,R.L. 801, 893
 Osaka,G. 1057
 Oshima,T. 39, 763
 Owens,R.J. 193

Panayotou,G. 527
 Pardanani,A. 593
 Pastan,I. 1323
 Pastor,N. 543
 Pawson,T. 609

Pederson,K. 91
 Pereboev,A.V. 167
 Ignat'ev,G.M. 167
 Pérez,S. 699
 Perez-Prat,E.M. 1153
 Permyakov,E.A. 63
 Petsko,G.A. 905, 1103
 Pettersson,K. 185
 Philippopoulos,M. 565
 Planas,A. 939
 Plückthun,A. 81
 Polticelli,F. 551
 Pomés,R. 663
 Poncin,A. 249
 Pons,J. 939
 Porstmann,T. 471
 Potete,A.R. 593
 Pratt,K.A. 13, 59
 Préaux,G. 249
 Pregel,M.J. 1309
 Price,S.L. 109

Querol,E. 939
 Quirk,D.J. 261

Raines,R.T. 261
 Rajalakshmi,N. 1039
 Raucci,G. 31
 Recktenwald,A. 835
 Reczko,M. 389
 Reed,C. 1233
 Rehberg,E.F. 293
 Reilly,P.J. 575
 Rein,R. 893
 Reiter,Y. 1323
 Revell,D.F. 59
 Ribó,M. 261
 Rice,D.W. 147
 Richelle,J. 647
 Ridgway,J.B.B. 1057
 Robben,J. 159
 Rollema,H.S. 117
 Rooman,M.J. 647, 849
 Rosenberg,S. 463
 Royer,Jr.,W.E. 593
 Rüker,F. 471
 Russell,R.J.M. 583
 Rutter,W.J. 261
 Ruysschaert,J.-M. 249
 Ryffel,G.U. 733

Sakurai,M. 763
 Salakoski,T. 501, 505
 Sampson,E. 1317
 Saqi,M. 1069
 Scandurra,R. 1287
 Schneider-Mergener,J. 471
 Schomburg,D. 45
 Schrag,J.D. 835
 Selbig,J. 339
 Shen,S.-H. 1309
 Shi,J. 193
 Shibata,M. 893
 Shoichet,B.K. 1017
 Siezen,R.J. 117
 Sigal,E. 275
 Simon,I. 417
 Sizmann,D. 725
 Skaper,S.D. 175
 Skolnick,J. 225

Sloane,D.L. 275
 Smalås,A.O. 379
 Smith,D.D.S. 13
 Smith,T.J. 1275
 Soares,C.M. 5
 Söderlund,H. 185, 725
 Solar,I. 717
 Soman,K.V. 397
 Soumillion,P. 451
 Stafford,III,W.F. 301
 Sternber,M.J.E. 513
 Stigler,R.-D. 471
 Stark,H.J. 1093
 Storer,A.C. 53, 1309
 Stratton-Thomas,J.R. 463
 Suck,D. 283
 Suhai,S. 389
 Summerford,C.M. 593
 Summers,N.L. 1215
 Sumner,I.G. 13
 Sun,S. 1205
 Sundaram,P.V. 1039
 Suns,S. 769
 Suske,G. 71
 Sutherland,J. 1317
 Sutton,B.J. 193
 Suyama,M. 1075
 Suzuki,M. 1, 319, 329, 1259
 Szardenings,M. 45
 Szilágyi,A. 779

Tai,M.-S. 301
 Takahashi-Fujii,A. 1171
 Takkinnen,K. 185, 725
 Tanaka,N. 763
 Tanaka,T. 711
 Tapia,O. 5
 Taylor,J.S. 1145
 Taylor,M.A.J. 59
 Teeri,T.T. 185, 443, 725
 Telemann,O. 185, 443, 1253
 Teo,B. 1145
 Thomas,D.Y. 835
 Thomas,P.D. 769
 Thomas-Soumarnon,A. 829
 Thornton,J.M. 127, 217, 1093
 Toda,K. 1093
 Tomizawa,H. 1023
 Tramontano,A. 31, 403
 Trosset,J.-Y. 1029
 Tsai,C.-J. 981
 Turley,S. 153
 Tusnády,G. 417
 Tusnády,G.E. 417

Uchiyama,H. 1153
 Ueda,T. 201
 Uemori,T. 1171
 Uhlén,M. 601
 Urwin,P.E. 1303

Vajda,S. 1081
 Vakser,I.A. 371
 van Aalten,D.M.F. 1129
 Van der Schueren 159
 vanderSpek,J.C. 1317
 Vasel,B. 45
 Vehniäinen,M. 185
 Verhasselt,P. 159
 Verheijen,J.H. 293, 1295

Verkhivker,G. 677
 Vernet,T. 835
 Vervoort,J. 451
 Viihinen,M. 501, 505
 Villafranca,J.E. 677
 Villoutreix,B.O. 1253
 Vince,J.W. 843
 Volckaert,G. 159
 von Heijne,G. 693
 von Strandmann,E.P. 733
 von Strandmann,R.P. 733
 Voss,E.W. 749
 Vriend,G. 71

Walker,B. 491
 Wallace,A. 31
 Wallace,A.C. 127
 Wallin,E. 693
 Walshaw,J. 109
 Wang,X.-g. 147
 Warren,G.L. 905
 Warwicker,J. 1243
 Watanabe,K. 1153
 Waterfield,M.D. 527
 Weber,I.T. 1233
 Weiner,L.M. 301
 Weinhold,E.G. 457
 Weinstein,H. 543
 Weng,Z. 1081
 Werge,T.M. 403
 Westhead,D.R. 1197
 White,C.E. 1177
 White,L.R. 1177
 Whitlow,M. 749
 Widersten,M. 1163
 Willson,R.C. 663, 915
 Wilmanns,M. 627
 Wilson,D.B. 1145
 Wilson,K.P. 1017
 Wodak,S.J. 647, 849
 Wolf,E. 283
 Wolfson,H. 981
 Wong,W.L.T. 1057
 Wood,J.F. 749
 Wu,J. 1233

Xiang,Y. 565
 Xue,Y.-N. 1233

Yagi,N. 319, 329, 1259
 Yamada,H. 201, 1023
 Yamagishi,A. 39, 763
 Yamato,I. 935
 Yilmaz,S. 1163
 Yokel,E.M. 261
 Young,R.J. 193
 Youvan,D.C. 237

Zapata,G. 1057
 Závodszky,P. 779
 Zawadzke,L.E. 1275
 Zhang,C.-T. 425
 Zhang,X.-j. 1017
 Zhu,Z.-Y. 103
 Ziomek,E. 835
 Zoidl,C. 733
 Zvelebil,M.J.J.M. 527

Subject index

Accessible surface area used to estimate hydrophobic effect 437

Acetylcholine receptor cassette mutagenesis of acetylcholine binding site 143

Active site of *Clostridium symbiosum* glutamate dehydrogenase, site-directed mutagenesis 147

α_{1B} -Adrenergic receptor molecular dynamics simulation of signal transduction in 557

Alcaligenes faecalis pseudoazurin interaction with nitrite reductase, effect of site-directed mutagenesis 153

Alcohol dehydrogenase *Sulfolobus solfataricus*, thermostability, effect of mutation 31 yeast, site-directed mutagenesis 457

Alginate synthesis *Pseudomonas*, regulation of 63

Algorithm for identifying domains of proteins 513

Algorithms for dealing with gaps in protein sequence comparison 1075

Alkaline phosphatase *E. coli* D153G mutant of 865

Amino acid analogues incorporation of 7-azatryptophan into lysozyme 451

Amino acids determining hydrophobicity parameters 1081 relationships based on protein building features 417

Aminoacyl tRNA binding site-directed mutagenesis of elongation factor Tu 1267

α -Amylase *Bacillus licheniformis*, altering thermostability of 1029

Anti-receptor antibody crystal structure of OPG2 fragment 823

Antibodies artificial, strategy for constructing 601 bacterial secretion of mouse IgM Fab fragment 859 engineering disulphide-linked single-chain Fv dimers 301 engineering linear F(ab')₂ fragments 1057 improving labelling properties of anti-HAFP antibody Fab fragment 185 prediction of hypervariable CDR-H3 loop using neural network 389 recombinant, mutations affecting folding 81 stabilizing Fv fragments by engineering disulphide bonding 1323

Antibody-antigen binding free energy simulations of HyHEL-10/HEL complex 663 interaction of anti-HIV-1 gp41 Fab fragment with its peptide epitope 471 p*K_a* of HyHEL-5-hen egg lysozyme complex 915

Antimicrobial peptides based on *Staphylococcus aureus* δ -toxin 315

L-Arabinose isomerase *E. coli* 1189

Arachidonic acid positional specificity of lipoxygenase binding 275

Arc binding to DNA 1

Archaea *Pyrococcus furiosus* citrate synthase 583

Asparagine application of hydrogen bonding analysis in X-ray crystallography to orientate side chains 217

Aspartyl bonds in *Aspergillus awamori* glucoamylase, site-directed mutagenesis of 575

Aspergillus deletion analysis of glucoamylase starch-binding domain 1049

7-Azatryptophan incorporation into lysozyme 451

Bacillus caldothermophilus DNA polymerase, amino acid sequence required for 5'→3' exonuclease activity 1171

Bacillus licheniformis α -amylase, altering thermostability of 1029 1,3,1,4- β -glucanase, role of disulphide bond in stability of 939

Bacillus stearothermophilus lactate dehydrogenase, molecular dynamics simulation of protein loop closure 565

Bacillus subtilis isopropylmalate dehydrogenase, thermostability of chimera with *Thermus thermophilus* enzyme 39 subtilisin E, crystal structure of complex with phenylmethanesulphonyl fluoride 211

Barnase *in vivo* detection of low-activity mutants 497

α/β -Barrel structural stability, effect of β -residue packing 249

(α/β)₈-Barrel enzymes evolutionary relationships of 809

c-ErbB-2 (sFv')₂ version of monoclonal antibody against 301

C4b-binding protein interaction with protein S 1253

Calpain II recombinant, improving expression of 843

Cam and Tet, DNA binding domains of 1259

CAP DNA bending by 329

Carbonic anhydrase II structure of His94→Asp mutant 975

Cassette mutagenesis efficient design of combinatorial library 143 of *E. coli* trp repressor 935

Catalytic triad Cys-His-Asp, in dienelactone hydrolase 135 of *Geotrichum candidum* lipase 835

Cathepsin B alteration of subsite specificity by mutation 53

Cavities within globular proteins, detection of 1011

Cellulases *Thermomonospora fusca* endocellulase E2, modelling substrate binding 1145

Cellulose-binding domain fungal, molecular dynamics simulation of 443

Cephalosporins third generation, hydrolysis by engineered *Staphylococcus aureus* β -lactamase 1275

Chloramphenicol acetyltransferase reactivation of misfolding mutant as strategy for positive selection 159

Chymotrypsin inhibitor 2 solution structure 1117

Ciliary neurotrophic factor fusion protein with diphtheria toxin, characterization of 175

Citrate synthase from the hyperthermophile *Pyrococcus furiosus* 583

Classification of proteins by complete linkage clustering [letter] 501

Clostridium difficile glutamate dehydrogenase 1287

Clostridium symbiosum site-directed mutagenesis of glutamate dehydrogenase active site 147

CLUSPROT for analysis of determinants of subtilisin thermostability 21

Co-operativity of proteins, model for investigating 593

Combinatorial cassette mutagenesis of *Rhodobacter capsulatus* LH2 light-harvesting protein 237

Combinatorial library efficient design of 143 solid-phase gene assembly strategy for constructing 601

Complete linkage clustering used to identify protein families [letter] 501

Complex formation docking algorithm for low-resolution structures 371

Subject index

Conformational search

minimum perturbation, for modelling mutant structure of triose phosphate isomerase 1103

Contact matrix

use for protein structure prediction 339

Covalent modification

alters thermostability of papain 1039
of α -haemolysin, restores pore-forming activity 491

Cystatin C

inhibition of cysteine proteases, residues affecting 53

Cystatins

role of N-terminal region of oryzacystatin I 1303

Cysteine proteases

alteration of subsite specificity by mutation 53
recombinant pro-regions of papain and papaya proteinase IV inhibit mature enzymes 59

Cysteine proteinase inhibitors

role of N-terminal region of oryzacystatin I 1303

Cystic fibrosis transmembrane conductance regulator

prediction of epitopes using molecular modelling 829

Cytochrome P450cam

molecular dynamics simulation of pentachloroethane dehalogenation by 801

Dead-end elimination

for determining global minimum energy conformation 815
using fuzzy end elimination algorithm 893

Dehalogenation

of pentachloroethane by cytochrome P450cam 801

Dialysis

for effective renaturation of urea-denatured lysozyme 201

Dienelactone hydrolase

substrate-induced activation of 135

Digoxin

(sFv')₂ version of monoclonal antibody against 301

Diphtheria toxin

fusion protein with ciliary neurotrophic factor, characterization of 175

fusion with simian interleukin 15 1317

Distantly related proteins

protein sequence comparison of 1075

Disulphide bonding

for stabilizing Fv fragments 1323

role in stability of 1,3-1,4- β -glucanase 939

DNA bending

by CAP 329

DNA binding domains

of Cam and Tet 1259

DNA binding proteins

DNA recognition by helix-turn-helix proteins 329

interaction of transcription factors with DNA [review] 319

β -sheet, binding to DNA 1

DNA binding specificity

electrostatic analysis of TATA box binding protein mutants 543

DNA polymerase

Bacillus caldovenax, amino acid sequence required for 5' \rightarrow 3' exonuclease activity 1171

DNase I

interaction with DNA, altering sequence selectivity 283

Docking

algorithm for low-resolution structures 371

Domain-domain interaction

in tissue-type plasminogen activator hybrids with urokinase-type plasminogen activator 1295

Domains

algorithm for identifying 513

Double dynamic programming

compared with iterative algorithm 1197

Elastase inhibitors

comparison of predictive strategies for protein design 45

Electrostatic analysis

of TATA box binding protein mutants 543

Electrostatic interactions

algorithm for calculation of multiple site titration curves 243

Electrostatic potential field

of Cu,Zn superoxide dismutase 551

Electrostatics

determining pK_a of HyHEL-5-hen egg lysozyme complex 915
model for interaction of water with phenylalanine 109
molecular modelling of xylose isomerase catalysis 925
role in C4b-binding protein interaction with protein S 1253

Elongation factor Tu

site-directed mutagenesis 1267

Endocellulase E2

Thermomonospora fusca, modelling substrate binding 1145

Endoplasmic reticulum

determinants of zein retention in 91

Enzymes

classification by thermodynamic parameters 791

Epitopes

of cystic fibrosis transmembrane conductance regulator, prediction of using molecular modelling 829

Escherichia coli

cassette mutagenesis of *trp* repressor 935

magnesium binding by mutant alkaline phosphatase 865

Evolution

of sugar isomerases 1189

Evolutionary relationships

of $(\alpha\beta)_8$ -barrel enzymes 809

5' \rightarrow 3' Exonuclease

activity of *Bacillus caldovenax* DNA polymerase, amino acid sequence required for 1171

Expression vector

for phage display 1063

F(ab')₂ fragments

linear, engineering 1057

Fab fragment

expression vector for phage display 1063

of anti-hAHP antibody, improving labelling properties 185

of mouse IgM, bacterial secretion of 859

α -Fetoprotein

improving labelling properties of anti-hAHP antibody Fab fragment 185

Fibronectin

crystal structure of cell-binding type III module 823

Fluorescein

crystal structure of anti-fluorescein Fab 749

Four-helix bundle protein

as candidate vaccine against HIV 167

v-Fps

kinase domain of 609

Free energy calculations

of ligand-protein complexes 677

Free energy simulations

of HyHEL-10/HEL antibody-antigen binding 663

Fusion protein

diphtheria toxin-CNTF, characterization of 175

Fuzzy classification

for prediction of secondary structure 505

Fuzzy clustering

for predicting structural classes of proteins 425

Fuzzy end elimination

algorithm for finding global energy minimum 893

Fv dimers

disulphide-linked single-chain, engineering 301

Fv fragments

stabilizing by engineering disulphide bonding 1323

G-protein coupled receptors

model of binding site in substance P receptor and anti-SP antibody 403
N-terminal tails of 693

Gaps

in protein sequence comparison, algorithms for dealing with 1075

Gene inversion

as basis for *in vivo* detection of low-activity barnase mutants 497

Genetic algorithm

for predicting tertiary structure 769

for protein structure comparison 873

Geotrichum candidum

lipase, redesigning active site of 835

Global minimum energy conformation
 attaining, effect of temperature 883
 determining using dead-end elimination 815
 finding using fuzzy end elimination algorithm 893

Globular proteins
 detection of cavities within 1011
 predicting structural classes using fuzzy clustering 425

1,3-1,4- β -Glucanase
Bacillus licheniformis, role of disulphide bond in stability of 939

Glucoamylase
Aspergillus, deletion analysis of starch-binding domain 1049
Aspergillus awamori, site-directed mutagenesis of thermolabile aspartyl bonds in 575

Glutamate dehydrogenase
Clostridium symbiosum, site-directed mutagenesis of active site 147
Pyrococcus furiosus and *Clostridium difficile*, effects of domain swapping 1287

Glutamine amidotransferase
 predicting secondary structure 535

Glutathione synthetase
E.coli, site-directed mutagenesis of 711

Glutathione transferase A1-1
 creating nickel binding site by site-directed mutagenesis 1163

D-Glyceraldehyde-3-phosphate dehydrogenase
Thermotoga maritima, structural basis for thermostability 779

Glycosylation
 effect of elimination of glycosylation sites on human IgE Fc region binding to IgE receptors 193
 of ribonuclease A expressed in *S.cerevisiae* 261
 stereochemistry of *N*-glycosylation sites 699

Greek key jellyroll
de novo design of β -sheet 13

Growth hormone
 interaction with receptor 1215

GTPase mechanism
 of elongation factor Tu 1267

Haemoglobin
 dimeric, bacterial expression of 593

α -Haemolysin
 pore-forming activity restored by covalent modification 491

Haemolytic activity
 of *Staphylococcus aureus* δ -toxin, determinants of 315

Helical proteins
 with stable folds, design of 97

α -Helix
 composition of in thermophiles 905

Helix-turn-helix proteins
 DNA recognition by 329

HisA
 inverse protein folding by residue pair preference profile method 627

Histidine
 application of hydrogen bonding analysis in X-ray crystallography to orientate side chains 217

Histidine tag
 to aid purification of recombinant calpain II 843

Histidine-tagged proteins
 monoclonal antibody for detecting [Protocol] 733

Histone-like proteins
 binding of (AAKP)_n and (KKSP)_n to DNA 63

HIV
 four-helix bundle protein as candidate vaccine 167

HIV-1
 binding free energy of proteinase inhibitor 1137
 interaction of anti-HIV-1 gp41 Fab fragment with its peptide epitope 471
 predicting binding affinity of protease 677

HMG box protein
 homology modelling of Sox-5 615

Homology modelling
 determining global minimum energy conformation using dead-end elimination 815
 for analysis of thermostability 779
 of Sox-5 HMG box protein 615
 of tumour necrosis factor α receptor binding 1233
 of vicilin solubility 1243

Homology studies
 amino acid relationships based on protein building features 417

Hydrogen bonding
 application of hydrogen bonding analysis in X-ray crystallography to orientate side chains 217

Hydrophobic core
 designing sequences to fold with 1205
 of α -lactalbumin, effect of mutation 1153

Hydrophobic effect
 estimating 437
 model for interaction of water with phenylalanine 109

Hydrophobicity parameters
 of amino acids, determining 1081

Immunoassay
 improving labelling properties of anti-hAFP antibody Fab fragment 185

Immunoglobulin E
 effect of elimination of glycosylation sites on human IgE Fc region binding to IgE receptors 193

Immunotoxin
 recombinant ricin, expression and secretion from myeloma 481

Interleukin 15
 simian, fusion with diphtheria toxin 1317

Inverse protein folding
 by residue pair preference profile method 627
 designing sequences to fold with hydrophobic cores 1205

Inverse protein folding problem, 409

3-Isopropylmalate dehydrogenase
 altering thermostability using site-directed mutagenesis 763

Isopropylmalate dehydrogenase
 thermostability of *Thermus thermophilus* chimera with *Bacillus subtilis* enzyme 39

Iterative algorithm
 compared with double dynamic programming 1197

Kringle 2 domain
 effect of position in tissue-type plasminogen activator 293

α -Lactalbumin
 effect of mutation in hydrophobic core 1153

β -Lactamase
Staphylococcus aureus, engineered to hydrolyse third generation cephalosporins 1275

Lactate dehydrogenase
Bacillus stearothermophilus, molecular dynamics simulation of protein loop closure 565

Lactococcus lactis
 homology modelling of nisin–NisP interaction 117

Leader peptides
 homology modelling of nisin–NisP interaction 117

Ligand–protein interaction
 predicting binding affinity of HIV-1 protease 677

Ligand–receptor interaction
 docking algorithm for low-resolution structures 371

Light-harvesting protein
Rhodobacter capsulatus LH2, combinatorial cassette mutagenesis 237

LIGPLOT
 for 2-D representation of protein–ligand interaction 127

Linker modification
 effect of linker modification on molecular stability of single chain antibody 717

Lipase
Geotrichum candidum, redesigning active site of 835
 human pancreatic, catalytic triad of 835

Lipoxygenase
 positional specificity, effect of site-directed mutagenesis 275

Long loops
 role in protein folding 1093

Low complexity sequences
 structural analysis of 1069

Lysozyme
 free energy simulations of HyHEL-10/HEL antibody–antigen binding 663
 hen egg-white, enhancing thermostability 1023
 incorporation of 7-azatryptophan 451

Subject index

pK_a of HyHEL-5–hen egg lysozyme complex 915
T4, enhancing thermostability of 1017
urea-denatured, effective renaturation of 201

M3-muscarinic receptor
molecular dynamics simulation of signal transduction in 557

Magnesium binding
by *E. coli* D153G mutant alkaline phosphatase 865

Membrane proteins
N-terminal tails of G-protein coupled receptors 693

MetJ
binding to DNA 1

Mnt
binding to DNA 1

Molecular dynamics simulation
for investigating solution structure of chymotrypsin inhibitor 2 1117
of cellular retinol binding protein 1129
of enzyme-catalysed pentachloroethane dehalogenation 801
of fungal cellulose-binding domain 443
of HIV-1 protease inhibitor 1137
of pore closing in porin 5
of protein loop closure 565
of signal transduction in α_{1B} -adrenergic receptor and m3-muscarinic receptor 557
used to study mobility of bovine and salmon trypsin 379

Molecular modelling
for prediction of cystic fibrosis transmembrane conductance regulator epitopes 829

Molten globule state
of α -lactalbumin, stability of 1153

Monoclonal antibody
for detecting histidine-tagged proteins [Protocol] 733

Monte Carlo optimization
for protein side-chain prediction 363

Monte Carlo simulation
of protein folding 883

Multiple linkage clustering
for protein structure comparison 647

Myeloma
expression and secretion of recombinant ricin immunotoxin 481

Neural network
for protein side-chain contact mapping 225
for protein side-chain prediction 363
used for prediction of hypervariable CDR-H3 loop 389

Nickel binding site
in glutathione transferase A1-1, creating by site-directed mutagenesis 1163

Nisin
homology modelling of nisin–NisP interaction 117

Nitrite reductase
interaction with pseudoazurin, effect of site-directed mutagenesis 153

Oryzacystatin I
role of N-terminal region in cysteine proteinase inhibition 1303

P450-containing monooxygenase systems
structural domains of [Review] 737

Packing defects, 1011

Papain
and papaya proteinase IV, recombinant pro-regions inhibit mature enzymes 59
covalent modification alters thermostability 1039

Papaya proteinase IV
and papain, recombinant pro-regions inhibit mature enzymes 59
residues affecting inhibition of by cystatin C 53

Pentachloroethane
dehalogenation by cytochrome P450cam 801

Peptide–DNA binding
binding of (AAKP)_n and (KKSP)_n to DNA 63

Peptide epitope library
used to study interaction of anti-HIV-1 gp41 Fab fragment with its peptide epitope 471

Phage display
expression vector for 1063

Phagemid display
of urokinase plasminogen activator EGF-like domain 463

Phenylalanine
model for interaction with water 109

Phenylmethanesulphonyl fluoride
crystal structure of complex with subtilisin E 211

Phosphopeptides
analysis of interaction with SH2 domain 527

Pichia pastoris
expression system for human thrombomodulin 1177

pK
calculation of:algorithm for calculation of multiple site titration curves 243

Pore
 α -haemolysin pore-forming activity restored by covalent modification 491
predicting secondary structure of potassium channel H5 pore 397

Pore closing
in porin, mechanism of 5

Porin
mechanism of pore closing 5

Positional specificity
of lipoxygenase, effect of site-directed mutagenesis 275

Positive selection
using reactivation of chloramphenicol acetyltransferase misfolding mutant 159

Potassium channel
predicting secondary structure of H5 pore 397

Pro-regions
of papain and papaya proteinase IV, inhibit mature enzymes 59

Probability alignment, 999

Progesterone
model for binding to uteroglobin 71

Prolactin
human, interaction with receptor 1215

Protease
HIV-1, predicting binding affinity of 677

Protease inhibitors
comparison of predictive strategies for protein design 45

Protein–DNA interaction
interaction of transcription factors with DNA [review] 319

Protein–ligand interaction
2-D representation using LIGPLOT 127

Protein–protein interaction
pseudoazurin interaction with nitrite reductase, effect of site-directed mutagenesis 153

Protein Data Bank
structural classes within 981

Protein design
de novo design of Greek key jellyroll motif 13
of elastase inhibitors 45
of four-helix bundle protein as candidate vaccine against HIV 167
of helical proteins with stable folds 97

Protein families
classification by complete linkage clustering [letter] 501

Protein folding
database-derived potentials for [Review] 849
estimating hydrophobic effect 437
inverse protein folding problem 409
Monte Carlo simulation of 883
mutations affecting folding of recombinant antibodies 81
role of long loops 1093

Protein loop closure
molecular dynamics simulation of *Bacillus stearothermophilus* lactate dehydrogenase loop 565

Protein S
interaction with C4b-binding protein 1253

Protein sequence comparison
of distantly related proteins 1075

Protein side-chain contact mapping
using neural network 225

Protein side-chain prediction
using neural network and simulated annealing 363

Protein structure
comparing using spatial arrangement of secondary structure elements 353

Protein structure classification
algorithms for 981

Protein structure comparison
by multiple linkage clustering 647
genetic algorithm for 873

Protein structure prediction
by threading method 1197
database-derived potentials for protein folding [Review] 849
genetic algorithm for predicting tertiary structure 769
of hypervariable CDR-H3 loop, using neural network 389
predicting secondary structure of glutamine amidotransferase 535
predicting secondary structure of potassium channel H5 pore 397
predicting structural classes using fuzzy clustering 425
prediction of secondary structure using fuzzy classification 505
using contact matrix 339

Protein targeting
determinants of zein retention in endoplasmic reticulum 91

Protein tyrosine phosphatase 1C
regulation of 1309

Proteinase inhibitor
HIV-1, binding free energy of 1137

Pseudoazurin
interaction with nitrite reductase, effect of site-directed mutagenesis 153

Pseudomonas
regulation of alginate synthesis 63

Pyrococcus furiosus
citrate synthase 583
glutamate dehydrogenase 1287

Reaction rate
of enzymes, relationship with substrate specificity 791

Receptor binding
by prolactin and growth hormone 1215
by tumour necrosis factor α 1233

Renaturation
effective renaturation of urea-denatured lysozyme 201

Residue pair preference profile
for inverse protein folding 627

Retinol binding protein
cellular, molecular dynamics simulation of 1129

RGD molecules
common molecular scaffold for 823

Rhodobacter capsulatus
combinatorial cassette mutagenesis of LH2 light-harvesting protein 237

Ribonuclease
in vivo detection of low-activity barnase mutants 497

Ribonuclease A
cDNA cloning and mutagenesis 261

Ricin
expression and secretion of recombinant immunotoxin from myeloma 481

Scapharca
bacterial expression of dimeric haemoglobin 593

Secondary structure
evaluating methods for prediction of 103
of glutamine amidotransferase, predicting 535
prediction of using fuzzy classification 505

Secondary structure elements
spatial arrangement of, used to compare protein structure 353

Secretion
bacterial, of mouse IgM Fab fragment 859
of whole human IgE Fc region 193

Seed storage proteins
vicilin 1243

Sequence alignment
999

Sequence homology
method for deriving substitution matrix 641

Sequence selectivity
of DNase I interaction with DNA, altering 283

Serine proteases
Cys-His-Asp catalytic triad in dienelactone hydrolase 135
homology modelling of nisin-NisP interaction 117

SH2 domain
analysis of interaction with phosphopeptides 527

β -Sheet
de novo design of Greek key jellyroll motif 13
experimental test of predicted stability parameters [letter] 207
interaction with DNA 1

Signal transduction
in α_{1B} -adrenergic receptor and m3-muscarinic receptor, molecular dynamics simulation of 557

Simulated annealing
Monte Carlo optimization, for protein side-chain prediction 363

Single chain antibody
effect of linker alteration 725
effect of linker modification on molecular stability 717

Site-directed mutagenesis
effect on pseudoazurin interaction with nitrite reductase 153
of anti-HAHP antibody Fab fragment 185
of *Clostridium symbiosum* glutamate dehydrogenase active site 147
of *E.coli* glutathione synthetase 711
of elongation factor Tu 1267
of hen egg-white lysozyme 1023
of lipoxygenase, effect on positional specificity 275
of *Staphylococcus aureus* β -lactamase 1275
of thermolabile aspartyl bonds in *Aspergillus awamori* glucoamylase 575
of yeast alcohol dehydrogenase 457
to alter sequence selectivity of DNase I 283
to alter thermostability of α -amylase 1029
to create nickel binding site in glutathione transferase A1-1 1163
using to alter thermostability of 3-isopropylmalate dehydrogenase 763

Solid-phase gene assembly
strategy for constructing combinatorial library 601

Solute partitioning
for determining hydrophobicity parameters of amino acids 1081

Sox-5
homology modelling of 615

src homology 2 domains
role regulation of protein tyrosine phosphatase 1C 1309

Stability
experimental test of predicted β -sheet stability parameters [letter] 207

Staphylococcus aureus
 β -lactamase, engineered to hydrolyse third generation cephalosporins 1275
 δ -toxin, determinants of haemolytic activity 315

Starch-binding domain
of *Aspergillus* glucoamylase, deletion analysis 1049

Structural domains
of P450-containing monooxygenase systems [Review] 737

Substance P
model of binding site in receptor and anti-SP antibody 403

Substitution matrix
method for deriving 641

Substrate binding
Thermomonospora fusca endocellulase E2, modelling 1145

Substrate recognition
Clostridium symbiosum glutamate dehydrogenase, effect of site-directed mutagenesis of active site 147

Substrate specificity
of enzymes, relationship with reaction rate 791
of yeast alcohol dehydrogenase, altering using site-directed mutagenesis 457

Subtilisin E
crystal structure of complex with phenylmethanesulphonyl fluoride 211

Subtilisin
determinants of thermostability 21

Sugar isomerases
evolution of 1189

Sulfolobus solfataricus
alcohol dehydrogenase thermostability, effect of mutation 31

Superoxide dismutase
modelling 3-D structure of Cu,Zn SOD 551

Symmetry
4-fold and 8-fold, role in structural stability of α/β -barrel 249

T1M barrel proteins
glutamine amidotransferase predicted to have T1M barrel fold 535

T4
lysozyme, enhancing thermostability of 1017

Tandem repeats
binding of $(AAKP)_n$ and $(KKSP)_n$ to DNA 63

TATA box binding protein
electrostatic analysis of mutants 543

Tet
and Cam, DNA binding domains of 1259

Subject index

Thermodynamic parameters

classification of enzymes by 791

Thermobility

of aspartyl bonds in *Aspergillus awamori* glucoamylase 575

Thermomonospora fusca

endocellulase E2, modelling substrate binding 1145

Thermophiles

α -helix composition in 905

Thermostability

citrate synthase from the hyperthermophile *Pyrococcus furiosus* 583

determinants of in subtilisin 21

of hen egg-white lysozyme, enhancing 1023

of 3-isopropylmalate dehydrogenase, altering using site-directed mutagenesis 763

of papain, altering by covalent modification 1039

of *Pyrococcus furiosus* and *Clostridium difficile* glutamate dehydrogenase 1287

of *Sulfolobus solfataricus* alcohol dehydrogenase, effect of mutation 31

of T4 lysozyme, enhancing 1017

of *Thermotoga maritima* D-glyceraldehyde-3-phosphate dehydrogenase, structural basis 779

of *Thermus thermophilus* isopropylmalate dehydrogenase chimera with *Bacillus subtilis* enzyme 39

Thermotoga maritima

D-glyceraldehyde-3-phosphate dehydrogenase, structural basis for thermostability 779

Thermus thermophilus

isopropylmalate dehydrogenase, thermostability of chimera with *Bacillus subtilis* enzyme 39

Threading

method of protein structure prediction 1197

Threading algorithm

for addressing inverse protein folding problem 409

Three-helix bundle protein

surface mutagenesis of 601

Thrombomodulin

human, expression in *Pichia pastoris* 1177

Tissue-type plasminogen activator

effect of position of Kringle 2 domain 293

hybrids with urokinase-type plasminogen activator 1295

δ -Toxin

Staphylococcus aureus, determinants of haemolytic activity 315

Transcription factors

DNA binding domains of Cam and Tet 1259

interaction with DNA [review] 319

possible binding sites for TFIIA and TFIIB 543

TrAY

binding to DNA 1

Trichoderma reesei

cellulose-binding domain, molecular dynamics simulation of 443

Triose phosphate isomerase

modelling mutant structure 1103

trp repressor

E.coli, cassette mutagenesis of 935

Trypsin

bovine and salmon, mobility of, studied using molecular dynamics simulation 379

Tumour necrosis factor α

receptor binding 1233

Tyrosine protein kinase

kinase domain of v-fps 609

Urea

effective renaturation of urea-denatured lysozyme 201

Urokinase plasminogen activator

yeast expression and phagemid display of EGF-like domain 463

Urokinase-type plasminogen activator

hybrids with tissue-type plasminogen activator 1295

Uteroglobin

model for binding of progesterone 71

Vicilin

homology modelling of solubility 1243

X-ray crystallography

application of hydrogen bonding analysis to orientate side chains 217
of subtilisin E-PMSF complex 211

Xylose isomerase

molecular modelling of catalysis 925

Zein

determinants of retention in endoplasmic reticulum 91

Zinc binding site

in carbonic anhydrase II 975

of *Sulfolobus solfataricus* alcohol dehydrogenase, effect of mutation on thermostability 31

